LECTURE 7

DERIVATION OF DIFFERENCE APPROXIMATIONS USING UNDETERMINED COEFFICIENTS

• All discrete approximations to derivatives are linear combinations of functional values at the nodes

\[ f_i^{(p)} = \frac{a_\alpha f_\alpha + a_\beta f_\beta + \ldots + a_\lambda f_\lambda}{h^p} + E \]

• The total number of nodes used must be at least one greater than the order of differentiation \( p \) to achieve minimum accuracy \( O(h) \).

• To obtain better accuracy, you must increase the number of nodes considered.

• For central difference approximations to even derivatives, a cancelation of truncation error terms leads to one order of accuracy improvement
**Forward second order accurate approximation to the first derivative**

- Develop a forward difference formula for $f_i^{(1)}$ which is $E = O(h)^2$ accurate
- First derivative with $O(h)$ accuracy $\Rightarrow$ the minimum number of nodes is 2
- First derivative with $O(h)^2$ accuracy $\Rightarrow$ need 3 nodes

![Nodes](image)

- The first forward derivative can therefore be approximated to $O(h)^2$ as:

$$\left. \frac{df}{dx} \right|_{x = x_i} - E = \frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h}$$

- T.S. expansions about $x_i$ are:

$\quad f_i = f_i$

$\quad f_{i+1} = f_i + hf_i^{(1)} + \frac{h^2}{2}f_i^{(2)} + \frac{h^3}{6}f_i^{(3)} + O(h)^4$

$\quad f_{i+2} = f_i + 2hf_i^{(1)} + 2h^2f_i^{(2)} + \frac{4}{3}h^3f_i^{(3)} + O(h)^4$
• Substituting into our assumed form of $f_i^{(1)}$ and re-arranging

$$\frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h} = \frac{(\alpha_1 + \alpha_2 + \alpha_3)}{h} f_i$$

$$+ (\alpha_2 + 2\alpha_3) f_i^{(1)}$$

$$+ \left(\frac{\alpha_2}{2} + 2\alpha_3\right) h f_i^{(2)}$$

$$+ \left(\frac{1}{6} \alpha_2 + \frac{4}{3} \alpha_3\right) h^2 f_i^{(3)} + O(h)^3$$

• Desire $f_i^{(1)}$ and $2^{nd}$ order accuracy $\Rightarrow$ coefficient of $f_i^{(1)}$ must equal unity and coefficients of $f_i$ and $f_i^{(2)}$ must vanish

$$\frac{\alpha_1 + \alpha_2 + \alpha_3}{h} = 0$$

$$(\alpha_2 + 2\alpha_3) = 1$$

$$\left(\frac{\alpha_2}{2} + 2\alpha_3\right) h = 0$$
• Solving these simultaneous equations

\[ \alpha_1 = -\frac{3}{2}, \; \alpha_2 = 2, \; \alpha_3 = -\frac{1}{2} \]

• Thus the equation now becomes

\[
\frac{-\frac{3}{2} f_i + 2 f_{i+1} - \frac{1}{2} f_{i+2}}{h} = (0)f_i + (2-1)f_i^{(1)} + (0)f_i^{(2)} + \left(\frac{1}{6} \cdot 2 - \frac{4}{3} \cdot \frac{1}{2}\right)h^2 f_i^{(3)} + O(h^3)
\]

\[\Rightarrow \]

\[ f_i^{(1)} = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \frac{1}{3}h^2 f_i^{(3)} + O(h^3) \]

• The forward difference approximation of 2\textsuperscript{nd} order accuracy

\[ f_i^{(1)} = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + E \quad \text{where} \quad E = \frac{1}{3}h^2 f_i^{(3)} \]
Forward first order accurate approximation to the second derivative

- Derive the $O(h)$ forward difference approximations to $f_i^{(2)}$

- Second derivative $\Rightarrow$ 3 nodes for $O(h)$ accuracy

\[
f_i^{(2)} - E = \frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h^2}
\]

- Develop Taylor series expansions for $f_i$, $f_{i+1}$ and $f_{i+2}$, substitute into expression and re-arrange:

\[
\frac{\alpha_1 f_i + \alpha_2 f_{i+1} + \alpha_3 f_{i+2}}{h^2} = \frac{(\alpha_1 + \alpha_2 + \alpha_3)}{h^2} f_i
\]

\[
+ \left( \frac{\alpha_2 + 2\alpha_3}{h} \right) f_i^{(1)}
\]

\[
+ \frac{1}{2} (\alpha_2 + 4\alpha_3) f_i^{(2)}
\]

\[
+ (\alpha_2 + 8\alpha_3) \frac{h}{6} f_i^{(3)} + O(h)^2
\]
• In order to compute $f_i^{(2)}$ we must have:

$$\frac{1}{h^2}(\alpha_1 + \alpha_2 + \alpha_3) = 0$$

$$\frac{1}{h}(\alpha_2 + 2\alpha_3) = 0$$

$$\frac{1}{2}(\alpha_2 + 4\alpha_3) = 1$$

⇒

$$\alpha_1 = 1, \quad \alpha_2 = -2, \quad \alpha_3 = 1$$

• Therefore

$$f_i^{(2)} = \frac{1}{h^2}(f_{i+2} - 2f_{i+1} + f_i) + E \quad \text{where} \quad E = - hf_i^{(3)}$$
**Skewed fourth order accurate approximation to the second derivative**

- Develop a fourth order accurate approximation to the second derivative at node $i$ which involves nodes $i-1$, $i$ and subsequent nodes to the right of node $i$

  $$ f_i^{(2)} \rightarrow \text{requires 3 nodes for } O(h) \text{ accuracy} $$

  $$ \rightarrow \text{requires 4 nodes for } O(h)^2 \text{ accuracy} $$

  $$ \rightarrow \text{requires 5 nodes for } O(h)^3 \text{ accuracy} $$

  $$ \rightarrow \text{requires 6 nodes for } O(h)^4 \text{ accuracy} $$

- Therefore we consider nodes

  $i-1 \quad i \quad i+1 \quad i+2 \quad i+3 \quad i+4$

- $f_i^{(2)}$ is approximated as:

  $$ f_i^{(2)} - E = \frac{\alpha_1 f_{i-1} + \alpha_2 f_i + \alpha_3 f_{i+1} + \alpha_4 f_{i+2} + \alpha_5 f_{i+3} + \alpha_6 f_{i+4}}{h^2} $$
• Steps to solve for the unknown coefficients in the linear combination for $f_i^{(2)}$

  • Develop Taylor series expansions for $f_{i-1}$, $f_{i+1}$, $f_{i+2}$, $f_{i+3}$, $f_{i+4}$

  • Substitute and re-arrange to collect terms on equal derivatives

  • Generate equations by setting coefficients of $f_i^{(2)}$ to 1 and the remaining 5 leading coefficients to zero
NUMERICAL DIFFERENTIATION USING DIFFERENCE OPERATORS

Difference Operators

First order difference operators

- Consider the following full and intermediate nodes

\[
\begin{array}{c}
\text{i-1} \quad \text{i} \quad \text{i+1} \\
\hline
\hline
\text{i-1/2} \quad \text{i+1/2}
\end{array}
\]

- First order forward difference operator

\[ \Delta f_i = f_{i+1} - f_i \]

- First order backward difference operator

\[ \nabla f_i = f_i - f_{i-1} \]

- First order central difference operator defined using full node functional values

\[ \delta f_i = f_{i+1} - f_{i-1} \]
Notes

• Intermediate functional values are defined as

\[ f_{i + \frac{1}{2}} = f(x_i + \frac{h}{2}) \]

• First order central difference operator defined using intermediate nodes

\[ \delta f_i = f_{i + \frac{1}{2}} - f_{i - \frac{1}{2}} \]

• The central difference operator is defined at an intermediate node as

\[ \delta f_{i + \frac{1}{2}} = f_{i + 1} - f_i \]

• The order of the difference operator is related to the number of times that the operator is applied and not to the order of accuracy

• Higher order difference operators \( \rightarrow \) simply repeat operation as indicated by the operator
Second order forward difference operator

\[ \Delta^2 f_i = \Delta(\Delta f_i) \]

\[ = \Delta(f_{i+1} - f_i) \]

\[ = \Delta f_{i+1} - \Delta f_i \]

\[ = (f_{i+2} - f_{i+1}) - (f_{i+1} - f_i) \]

\[ \Delta^2 f_i = f_{i+2} - 2f_{i+1} + f_i \]
**Third order backward difference operator**

\[ \nabla^3 f_i = \nabla^2 (\nabla f_i) \]

\[ = \nabla^2 (f_i - f_{i-1}) \]

\[ = \nabla (\nabla f_i - \nabla f_{i-1}) \]

\[ = \nabla [(f_i - f_{i-1}) - (f_{i-1} - f_{i-2})] \]

\[ = \nabla [f_i - 2f_{i-1} + f_{i-2}] \]

\[ = \nabla f_i - 2\nabla f_{i-1} + \nabla f_{i-2} \]

\[ = (f_i - f_{i-1}) - 2(f_{i-1} - f_{i-2}) + (f_{i-2} - f_{i-3}) \]

\[ \nabla^3 f_i = f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3} \]
Second order central difference operator

\[ \delta^2 f_i = \delta(\delta f_i) \]

\[ = \delta \left( f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}} \right) \]

\[ = \delta f_{i+\frac{1}{2}} - \delta f_{i-\frac{1}{2}} \]

\[ = (f_{i+1} - f_i) - (f_i - f_{i-1}) \]

\[ \delta^2 f_i = f_{i+1} - 2f_i + f_{i-1} \]
**Second order mixed difference operator**

- We can also apply different operators; e.g.

\[ \nabla^{n-m}\Delta^m, \quad 1 \leq m \leq n \]

- Applying a first order forward difference operator and then a first order backward difference operator

\[
\nabla \Delta f_i = \Delta(\nabla f_i)
\]

\[
= \Delta(f_i - f_{i-1})
\]

\[
= \Delta f_i - \Delta f_{i-1}
\]

\[
= (f_{i+1} - f_i) - (f_i - f_{i-1})
\]

\[
\Delta \nabla f_i = f_{i+1} - 2f_i + f_{i-1}
\]

- We note that \( \delta^2 = \Delta \nabla = \nabla \Delta \) and in general \( \delta^{2m} = \nabla^m \Delta^m \rightarrow (2m)^{th} \) order central difference operator
Approximations to Differentiation Using Difference Operators

\[
\frac{df}{dx}\bigg|_{x_i} \approx \frac{\Delta f_i}{\Delta x_i}
\]

\[
\frac{df}{dx}\bigg|_{x_i} \equiv \frac{\nabla f_i}{\nabla x_i}
\]

\[
\frac{df}{dx}\bigg|_{x_i} \equiv \frac{\delta f_i}{\delta x_i}
\]

**First order backward difference operator approximation to the first derivative**

\[
f_i^{(1)} \equiv \frac{\nabla f_i}{\nabla x_i}
\]

\[
\nabla x_i = h
\]

\[
f_i^{(1)} = \frac{f_i - f_{i-1}}{h}
\]
**First order central difference operator approximation to the first derivative**

\[ f_i^{(1)} \equiv \frac{\delta f_i}{\delta x_i} \]

\[ f_i^{(1)} \equiv \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{h} \]

\[ \delta x_i = 2h \]

\[ f_i^{(1)} \equiv \frac{f_{i+1} - f_{i-1}}{2h} \]
Central difference approximation to the first derivative as an average of first order forward and backward difference approximations

• We note that first order central difference approximations can also be derived as arithmetic averages of first order forward and backward difference approximations

\[
f_i^{(1)} = \frac{1}{2} \left[ \frac{\Delta f_i}{\Delta x_i} + \frac{\nabla f_i}{\nabla x_i} \right]
\]

\[
f_i^{(1)} = \frac{1}{2} \left[ \frac{f_{i+1} - f_i}{h} + \frac{f_i - f_{i-1}}{h} \right]
\]

\[
f_i^{(1)} = \frac{f_{i+1} - f_{i-1}}{2h}
\]

• This concept can be generalized to central approximations to higher order derivatives as well (see the next section)
General difference operator approximations to derivatives

- In general we can approximate derivatives using
  - Forward approximations
    \[ f_i^{(p)} = \frac{\Delta^p f_i}{h^p} + O(h) \]
  - Backward approximations
    \[ f_i^{(p)} = \frac{\nabla^p f_i}{h^p} + O(h) \]
  - Central approximations
    \[ f_i^{(p)} = \frac{\nabla^p f_{i+\frac{p}{2}} + \Delta^p f_{i-\frac{p}{2}}}{2h^p} + O(h)^2 \quad p \text{ even} \]
    \[ f_i^{(p)} = \frac{\nabla^p f_{i+\frac{p-1}{2}} + \Delta^p f_{i-\frac{p-1}{2}}}{2h^p} + O(h)^2 \quad p \text{ odd} \]
• A complete operator approach to central differencing can be developed. However this approach is somewhat artificial and overly complicated.